# Clathrate & Inclusion compound

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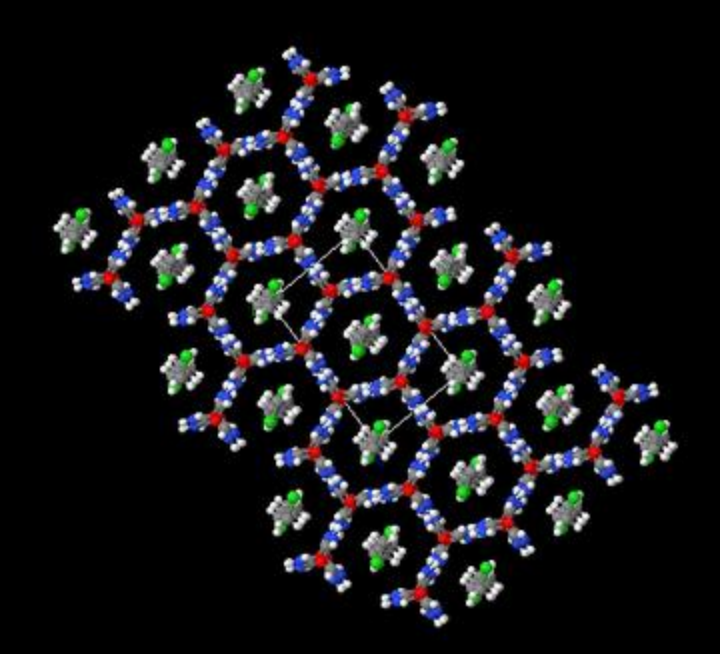
# Clathrate compound

•A **clathrate** is a chemical substance consisting of a lattice that traps or contains molecules.

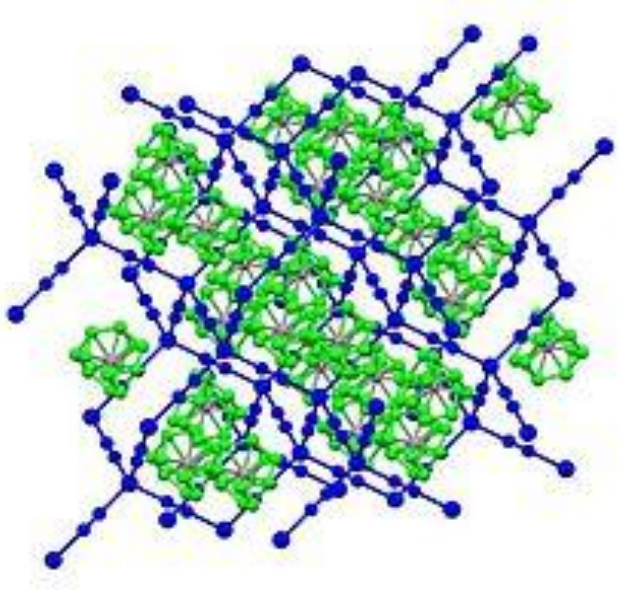
• The word *clathrate* is derived from the Latin *clatratus* meaning *with bars or a lattice*.

•Traditionally, clathrate compounds are polymeric and completely envelop the guest molecule, but in modern usage clathrates also include **host-guest complexes** and **inclusion compounds**.

•According to IUPAC, clathrates are "Inclusion compounds in which the guest molecule is in a cage formed by the host molecule or by a lattice of host molecules.



Structure of the 3:1 inclusion complex of urea and 1,6-dichlorohexane. The framework is composed of molecules of urea that are linked by hydrogen bonds, leaving approximately hexagonal channels into which align the molecules of the chlorocarbon. Color scheme: oxygen is red, nitrogen is blue, chlorine is green.



Structure of the clathrate consisting of cadmium cyanide host and carbon tetrachloride guest, $Cd(CN)_2 \cdot CCl_4$. Blue = $Cd(CN)_2$ framework, gray = C, green = disordered Cl.

# Clathrate/Inclusion Compounds

- A chemical substance consisting of a lattice of one type of crystal structure trapping and containing a second type of molecule. Therefore, a clathrate is a material which is a weak composite, in which molecules of suitable size are captured in spaces which are left by the other compounds.
- Molecules of one substance are completely enclosed within the crystal structure of another.

# Inclusion compound

- In host-guest chemistry, an **inclusion compound** is a complex in which one chemical compound (the "host") forms a cavity in which molecules of a second "guest" compound are located.

- The definition of inclusion compounds is very broad, extending to channels formed between molecules in a crystal lattice in which guest molecules can fit.

- If the spaces in the host lattice are enclosed on all sides so that the guest species is 'trapped' as in a cage, the compound is known as a clathrate.

- In molecular encapsulation, a guest molecule is actually trapped inside another molecule.

# INCLUSION COMPOUNDS

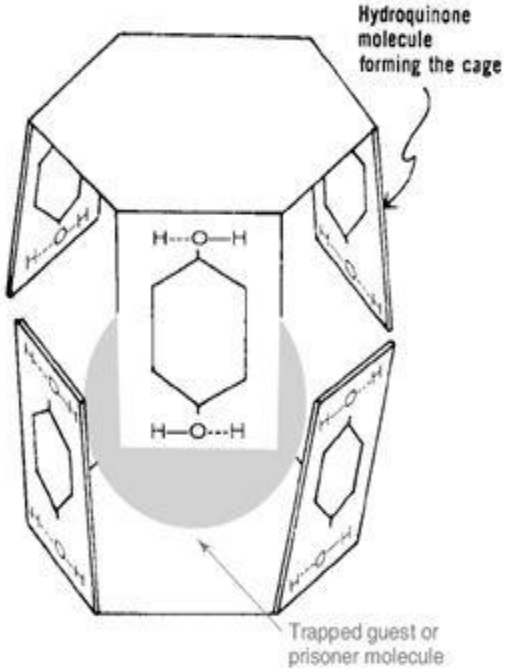
**Clathrates** – crystallize in a ***cage-like*** lattice in which the coordinating compound is entrapped. Molecular size of the encaged component is important. Examples are

**Hydroquinone crystals** that traps methanol, $CO_2$ and HCl but not smaller and larger molecules; and

**Warfarin sodium USP** is a clathrate of water, isopropyl alc and sodium warfarin.

# Clathrates

- **Coordinating compound is entrapped in the form of a cage-like lattice**
  - Molecular size of encaged components is important
- **Hydroquinone (quinol)**
  - Cage-like hydrogen-bonded structure
  - 4.2 Å hole
  - Entrap one small moelcule to every two quinol molecules
  - Molecules like MeOH, $CO_2$, HCl can be trapped but smaller molecules ($H_2$) and larger molecules (EtOH) cannot be accommodated
- **Warfarin sodium**



# Inclusion complexes

- **Inclusion (occlusion) complexes**
  - Compounds resulting more from architecture of molecules than from chemical affinity
  - Channel lattice type
  - Layer type
  - Clathrates
  - Monomolecular inclusion compounds: Cyclodextrins
  - Molecular sieves

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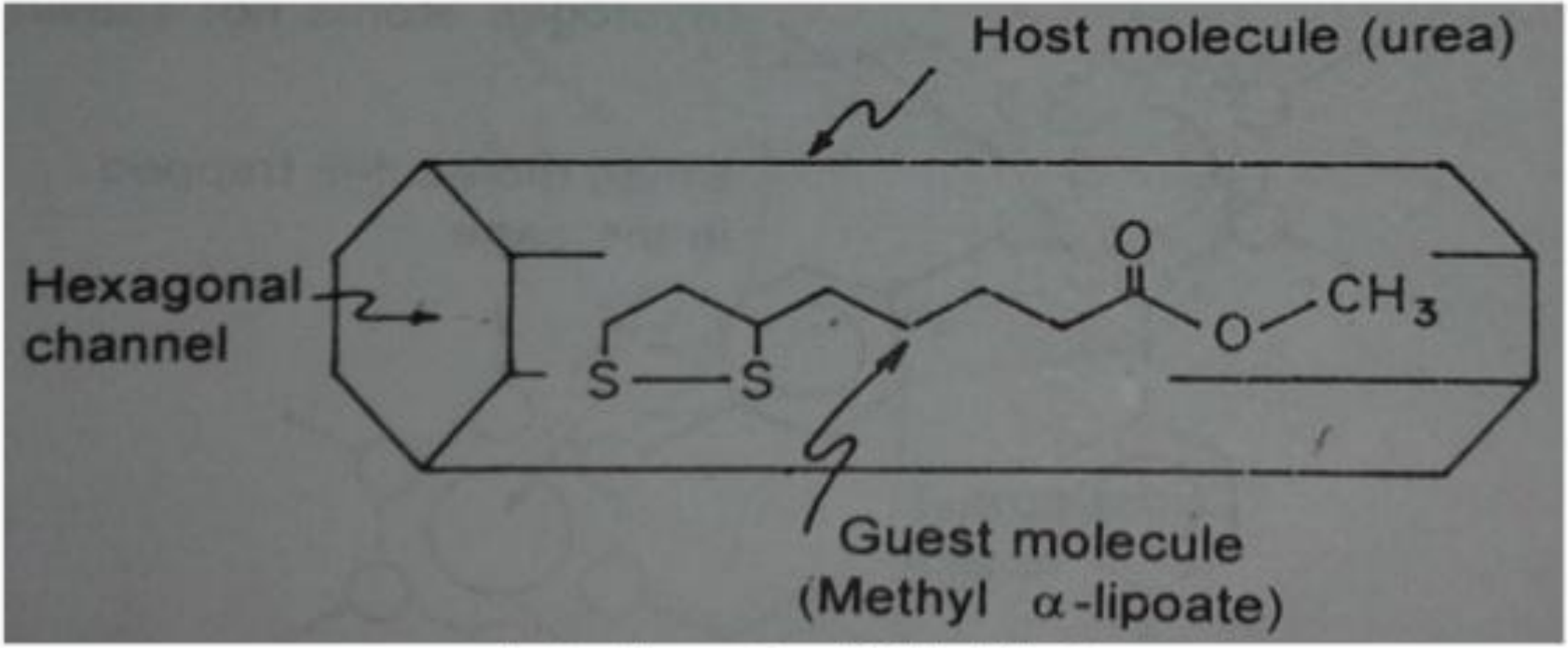
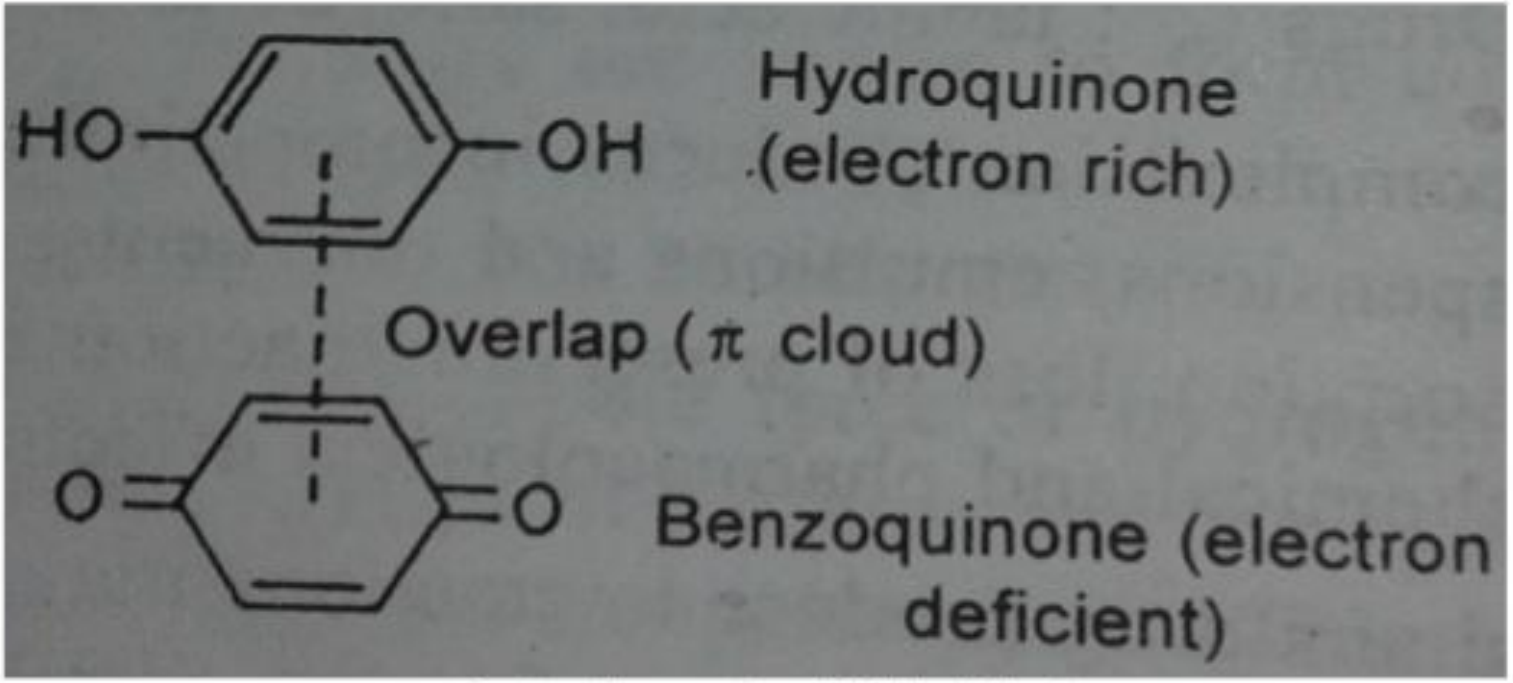
# 1. Channel types

- Channels are formed by crystallization of the host molecules, the guest component is usually limited to long, unbranched straight chain compounds.



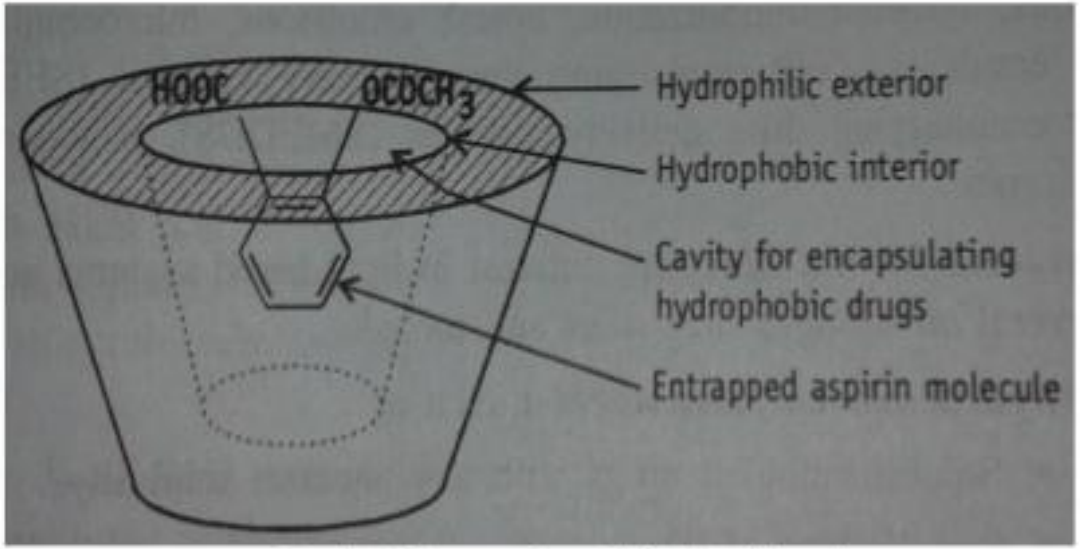
# 4. Quinhydrone types

- The molecular complex of this type is obtained by mixing alcoholic solutions of equimolar quantities of hydroquinone and benzoquinone.



# 4. Monomolecular types

- Monomolecular inclusion compounds involve the entrapment of a single guest molecule in the cavity of one host molecule.
- Most of the host molecules are cyclodextrins.
- The interior of the cavity is relatively hydrophobic, whereas the entrance of the cavity is hydrophilic in nature.



# Channel Hydrates Compound.x$H_2O$

- Hydrates in this class contain water in lattice channels, where the water molecules included lie next to other water molecules of adjoining unit cells along an axis of the lattice forming "channels" through the crystal.

| S.N. | Cage compounds(Clathrates) | Channel Compounds |
|---|---|---|
| 1 | Quinols | Urea complexes |
| 2 | Gas hydrates | Cyclodextrines |
| 3 | | Chloleic acid |
| 4 | | Biphenyl |

# General Methods of Preparation

- Crystallization of host in prescence of guest molecule.
- Urea complexes are prepared by mixing hot methanolic solution of urea and of the guest and allowing to crystallise upon cooling.
- The quinol-inert gas, clathrates are obtained by crystallising hydroquinone under pressure of the nobel gas.

# Uses

1. Resolution of Mixtures

I. Removal of straight chain hydrocarbons present in petroleum through urea complexation from HC mixture.

II. Removal of free fatty acids from oilnor waxws by treatment with moist urea.

III. Separation of saturated and unsaturated fattyacids by urea adduct formation.

IV. Cis-trans isomers can be separated by urea complexation.

V. Benzene can be separateed from the mixture of benzene and cyclohexane.

2. Storage of substances :

a)Certain substances can be protected for long time in form of inclulsion compounds. E.g. Auto oxidation of oleic acid does not occur when the acid is in form of urea complex.

b) The clathrates of inert gases provides a convenient method of dispersing the gases without restoring to high pressure cylinders.

Thank You